

NAG1-00030

Statistical Methods for Rapid Aerothermal Analysis and Design Technology: Validation

Final Report

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December 31, 2003

Abstract

The cost and safety goals for NASA's next generation of reusable launch vehicle (RLV) will require that rapid high-fidelity aerothermodynamic design tools be used early in the design cycle. To meet these requirements, it is desirable to identify adequate statistical models that quantify and improve the accuracy, extend the applicability, and enable combined analyses using existing prediction tools. The initial research work focused on establishing suitable candidate models for these purposes. The second phase is focused on assessing the performance of these models to accurately predict the heat rate for a given candidate data set. This validation work compared models and methods that may be useful in predicting the heat rate.

Introduction

There are two phases to this project and they are (1) model development and (2) model validation. This approach was aimed at identifying statistical/mathematical models that best characterize and/or model a set of sphere stagnation data (See Table 1). Once several candidate models were identified, they are tested in the second phase to see if they are able to predict heat rate values for a given smaller candidate data set within the normal trajectory of corridor values.

In the initial phase, five models for predicting heating rate within the entry corridor were identified. Comparisons of the adequacy of the models were made using R^2 (coefficient of determination), adjusted R^2 , standard error and F- statistic. In addition, graphical techniques like 3-D plots, contour plots, normal probability plots and residual analysis were used to better understand the relationship between the dependent and predictor variables. Some of the models including multiple linear regression, polynomial regression (quadratic and cubic), classification and regression trees (CART), Loess and Kriging models were investigated. The Loess and Kriging models were also explored during the second phase. Much of the initial phase work is summarized in a paper presented at the Annual Joint Statistical Meetings in August 2002 in New York City and is included in the Appendix.

The second phase was directed at model validation. Performance comparisons were conducted on a candidate data set to see which of the identified models best predicted the dependent variable, heat rate, with overall minimum percent error. In this approach, the identified models from the initial phase are used to predict heating rate for a smaller sphere stagnation test data set. This was followed by error analysis to determine which model produced overall minimum error.

Validation Approach

In this section, validation of identified models associated with the corridor data set is explored (See description in the Proceedingspaper in the Appendix). The validation process consisted of the following steps:

- (1) Use five identified models/methods on the candidate data set to obtain predicted heat rates for the respective models;
- (2) Calculate the percent (%) error [$100 * ((\text{actual} - \text{predicted}) / \text{actual})$] for each measurement in the data set for various models;
- (3) Identify the model or method that has consistent minimum percent error. For purposes of this study, a calculated percent error less than 5% is considered acceptable.

Description of Other Models

Loess

Loess was originally pioneered by Cleveland, W.S. (1979). Specifically, Loess denotes a method that is more descriptively known as locally weighted polynomial regression. It is one of many modern modeling methods that build on classical methods, such as linear and non-linear least squares regression. Modern regression methods are designed to address situations in which the classical procedures do not perform well. Loess combines much of the simplicity of linear least squares regression with the flexibility of nonlinear regression.

Assume that for $i = 1$ to n , the i^{th} measurement y_i of the response variable y and the corresponding measurement x_i of the vector x of p predictors are related by

$$y_i = g(x_i) + \varepsilon_i$$

where g is the regression function and ε_i is the random error. The idea of local regression is that near $x = x_0$, the regression function $g(x_i)$ can be locally approximated by the value of the function in some specified parametric class. Such approximation is obtained by fitting a regression surface to the data points within a chosen neighborhood of the point x_0 .

In the Loess method, weighted least squares is used to fit linear and quadratic functions of the predictors at the centers of neighborhoods. The radius of each neighborhood is chosen so that the neighborhood contains a certain percentage of the data points. The fraction of the percentage, called the smoothing parameter, in each local neighborhood controls the smoothness of the estimated surface. The larger values of the smoothing parameter produce the smoothest response functions. Data points in a given local neighborhood are weighted by a smooth decreasing function of their distance from the center of the neighborhood.

In this analysis, the Loess method was applied to the sphere test data set of 15 measurements and used to predict the associated heat rate values. The results are shown in Table 2.

Kriging Method

Kriging is an interpolation method named after a South African engineer named D. G. Krige. He developed the method in an attempt to more accurately predict ore reserves. Kriging is based on the assumption that the parameter being interpolated can be treated as a regionalized variable. A regionalized variable is intermediate between a truly random variable and a completely deterministic variable. It is assumed to vary in a continuous way from one location to the next and points that are near each other have a certain degree of spatial correlation. The points that are widely separated are assumed to be statistically independent (Cressie, 1993).

There are several Kriging methods including Simple, Ordinary, Zonal and Universal Kriging. Only the ordinary Kriging method will be reviewed in this report to provide further understanding of how the method works. The first step in ordinary Kriging is to construct a variogram from a data set to be interpolated. A variogram consists of two parts: experimental variogram and a model variogram. Suppose the value to be interpolated is referred to as f . The experimental variogram is found by calculating the variance (v) of each point in the data set with respect to each of the other points and plotting the variance versus the distance (h) between the points.

After the experimental variogram is computed, the next step is to define a model variogram. This variogram is a mathematical function that models the trend in the experimental variogram. When the model variogram is determined, it is used to compute the weights used in Kriging. The basic equation used in ordinary Kriging is as follows:

$$F(x,y) = \sum_{i=1}^n w_i f_i$$

Where n is the number of scatter points in the data set, f_i are the values of the scatter points and w_i are the weights assigned to each scatter point. The Kriging method was implemented using the Sufer 8 Software package and applied to the sphere test data set to predict heat rate values. The results of the analysis are provided in Table 2.

Surface-Fitting Method

The Table Curve 3D, marketed by SPSS of Chicago, IL, is mathematical software designed for Windows which fits and ranks built-in frequently encountered models. In highly automated processing steps, Table Curve 3D allows the user to quickly review the ideal fit for three dimensional data using pre-defined equation sets. The software includes, but is not limited to the following fitting options: Surface-Fit All, Surface-Fit Linear Equations, Surface-Fit Simple Equations, Surface-Fit Robust Plane, Surface-Fit Polynomial Equations and Surface-Fit Rational Equations.

In implementing anyone of the above options, Table Curve 3D will rank the pre-defined equation set according to following statistical measures: R^2 (Coefficient of Determination), DF (Degrees of Freedom) Adjusted R^2 , Fit Standard Error and F-value. Table Curve 3D was applied to the sphere test data set to predict heat rates values. The results of the analysis are provided in Table 2.

Prediction

Table 1 in the Appendix lists the 15 data measurements used to assess the models relating the response variable, heat rate and 10 predictor variables. The actual, predicted heat rate values and the calculated percent error values are provided in Table 2 below.

Table 1. Sphere Test Data Set

Velocity, ft/sec	Twall, deg R	Pressure, lb/ft ²	Density, slugs/ft ³	Temp, deg R	Mach	Dyn. Pres. lb/ft ²	Reynolds per ft	Energy, ft ³ /sec	Heat Rate, BTU/ft ² /s
2.500E+04	3.000E+03	5.84E-03	1.01E-08	3.36E+02	2.78E+01	3.16E+00	9.65E+02	1.58E+05	3.07E+01
2.350E+04	3.000E+03	7.65E-03	1.33E-08	3.36E+02	2.61E+01	3.66E+00	1.19E+03	1.72E+05	4.72E+01
2.100E+04	3.000E+03	7.54E-02	1.14E-07	3.84E+02	2.19E+01	2.52E+01	8.18E+03	1.06E+06	5.84E+01
1.750E+04	3.000E+03	2.36E-01	3.26E-07	4.21E+02	1.74E+01	5.00E+01	1.80E+04	1.75E+06	5.38E+01
1.300E+04	3.000E+03	6.71E-01	8.52E-07	4.59E+02	1.24E+01	7.20E+01	3.27E+04	1.87E+06	3.11E+01
9.000E+03	3.000E+03	1.77E+00	2.11E-06	4.87E+02	8.32E+00	8.55E+01	5.34E+04	1.54E+06	1.18E+01
6.500E+03	3.000E+03	4.65E+00	5.88E-06	4.60E+02	6.18E+00	1.24E+02	1.12E+05	1.62E+06	3.17E+00
4.500E+03	3.000E+03	1.36E+01	1.88E-05	4.21E+02	4.47E+00	1.90E+02	2.67E+05	1.71E+06	3.88E+00
2.540E+04	3.000E+03	3.31E-03	5.73E-09	3.36E+02	2.82E+01	1.85E+00	5.56E+02	9.39E+04	2.44E+01
2.250E+04	3.000E+03	5.84E-03	1.01E-08	3.36E+02	2.50E+01	2.56E+00	8.69E+02	1.15E+05	4.10E+01
2.050E+04	3.000E+03	1.07E-01	1.58E-07	3.95E+02	2.10E+01	3.33E+01	1.08E+04	1.36E+06	6.35E+01
1.450E+04	3.000E+03	3.35E-01	4.50E-07	4.33E+02	1.42E+01	4.74E+01	2.02E+04	1.37E+06	3.32E+01
1.200E+04	3.000E+03	1.10E+00	1.34E-06	4.78E+02	1.12E+01	9.64E+01	4.59E+04	2.31E+06	2.92E+01
6.500E+03	3.000E+03	3.45E+00	4.26E-06	4.72E+02	6.11E+00	9.01E+01	7.99E+04	1.17E+06	2.72E+00
3.250E+03	3.000E+03	1.86E+01	2.63E-05	4.11E+02	3.27E+00	1.39E+02	2.75E+05	9.02E+05	5.86E-01

Table 2. Performance Comparison of Five Models

	Actual	5V Model	CART	Table Curve	Kriging	Loess
1	30.73	30.45	22.88	30.43	32.23	31.24
2	47.23	39.95	45.54	47.57	47.37	47.88
3	58.4	56.28	63.89	58.38	59.16	58.23
4	53.81	52.98	51.03	53.47	55.21	55.13
5	31.11	33.3	26.9	31.06	30.9	32.39
6	11.8	14.71	15.59	13.36	11.93	12.81
7	3.17	3.15	3.91	6.2	2.77	6.13
8	3.88	-2.14	3.91	2.35	1.79	3.15
9	24.36	25.42	22.88	23.88	24.74	24.02
10	40.97	31.32	45.54	41.13	39.37	42.75
11	63.51	62.22	63.89	63.63	64.32	63.82
12	33.24	32.42	39.81	32.87	32.02	33.89
13	29.19	33.55	26.9	29.06	29.18	28.25
14	2.72	1.45	3.91	5.67	2.59	5.18
15	0.59	-0.1	3.91	0.85	0.72	0.34
% Error						
1		0.90%	25.55%	1.00%	-4.90%	-1.66%
2		15.40%	3.59%	-0.70%	-0.30%	1.38%
3		3.60%	-9.40%	0.00%	-1.30%	0.29%
4		1.50%	5.16%	0.60%	-2.60%	2.45%
5		-7.00%	47.36%	0.20%	0.70%	4.11%
6		-24.70%	-32.15%	-13.20%	-1.10%	8.55%
7		0.80%	-23.30%	-95.30%	12.70%	93.37%
8		155%	-74.00%	39.50%	53.90%	18.81%
9		-4.30%	6.09%	2.00%	-1.50%	1.39%
10		23.60%	-11.16%	-0.40%	3.90%	4.34%
11		2.00%	-0.60%	-0.20%	-1.30%	0.48%
12		2.50%	-19.77%	1.10%	3.70%	-1.95%
13		-15.00%	7.83%	0.40%	0.00%	3.22%
14		46.90%	-43.70%	-108.10%	4.90%	90.44%
15		117.60%	-562.46%	-45.10%	-23.20%	42.37%
	Actual	5V Model	CART	Table Curve	Kriging	Loess

Conclusions

Five models and/or methods were considered in the validation phase including classical multiple regression, classification and regression trees (CART), Table Curve, Kriging and Loess. Based on the performance criteria and the results in Table 2, Kriging performed better than the other methods in predicting heat rates for the Sphere Data Set in Table 1. Only three (3) of the Kriging predicted heat rate values exceeded the maximum 5% error (See Table 2). Loess and Table Curve both had five values that exceeded the 5% maximum error criterion as shown in Table 2. CART was the least effective at predicting heat rate values for the Sphere Test data set.

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APPENDIX

Multiple Regression Modeling of Aerothermal Data Sets

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KEY WORDS: Multiple Regression; Engineering Data Sets; Modeling; Prediction; Residual Analysis

This paper describes several regression analysis techniques used to analyze and model spherical stagnation heating data sets observed in aerothermal experiments. The objective is to identify statistical models that are suitable for modeling and prediction when using spherical stagnation heating data. Some of the regression techniques include classical multiple regression, best subset selection, classification and regression trees (CART), contour plots, 3-D plots and other graphical methods including residual plots. Comparisons are made to facilitate model selection.

Introduction

Recent designed experiments at NASA has demonstrated the need for considering higher fidelity aerodynamic heating early in the design cycle. In the experiment, the vehicle shape was optimized for aerodynamic performance and resulted in severe aerodynamic heating that forced costly redesign of the nose and wing surfaces and lowered flight margins. The availability of higher fidelity aerothermal analysis earlier in the design cycle could have prevented some of these problems.

There will be two phases to this project and they are model development and model validation. The initial phase will be to explore and/or develop the statistical and mathematical methods that can be used to transform the point wise aeroheating predictions of current tools to yield complete aerothermal environments through a trajectory corridor. The approach is intended to identify statistical and math models that best characterize and/or model a set of sphere stagnation data. Once several acceptable models and methods have been identified, they will be tested in the second phase to see if they are able to predict heating values within the normal trajectory of corridor values for minimum specified error.

Description of Sphere Stagnation Data Sets

There were two data sheets for analysis; one containing the full trajectory space (1269 measurements) and the second with measurements only within the entry

corridor (138 measurements). For these data sets, a sphere shape configuration is used and the measurements are taken at the stagnation point on the sphere. For simplicity, a sphere of one foot radius is assumed. Generally, as the sphere radius decreases, the heat rate measurements will increase.

For each case, eleven (11) variables are labeled on the worksheets. The first three variables (altitude, velocity, and wall temperature) are considered the basic independent variables. The other variables are derived from these basic three variables. For example, the density, pressure, and temperature are direct functions of altitude. The Mach number, dynamic pressure, Reynolds number, and energy variables are combinations of the 3 basic variables, e.g. dynamic pressure equals density*velocity*velocity. The response variable of interest is heat rate.

The heating rate values in the spreadsheet were generated using simple stagnation point calculations. The data sets contain values for velocity and altitude but no angle-of-attack values because of the sphere assumption.

Analysis Methods

Our goal is to begin with some rudimentary analysis on these type data sets to explore the behavior and relationships using correlations, summary statistics, graphics including contour plots and 3-D plots, robust and residual analyses. Several regression models were investigated including multiple linear regression, classification and regression trees (CART), best subset, quadratic and cubic regression models as well as some graphical methods. Regression analysis allows one to model the relationship between a response variable and one or more predictor variables. One of the useful features of a regression model is that it can be used to predict or estimate a future response value based on a given set of values of the predictor variables.

Regression analysis results usually include the following: regression equation, predictor table, summary statistics, ANOVA Table, list of unusual observations, contour plots, 3-D plots and residual plots. To appropriately use the t-test, F-test and associated confidence intervals, the data are assumed to meet certain conditions. These include (1) the residuals (error component) are assumed to be normally distributed, (2) variation is constant (homoscedasity) and (3) the measurements are independent. The study of unusual patterns in the residuals through residual analysis may indicate underlying weaknesses in the model.

Data Exploration

It should be noted that unless otherwise indicated tables and figures will appear in the Appendix. First the summary statistics for the independent and response variables were computed.

Prior to the model building activities, graphical methods were used to help identify any underlying relationships between the variables being studied. In particular, matrix plots of cross-graphs of the variables were generated. These plots showed:

- Apparent quadratic relationship between heat rate and altitude, temperature
- Strong linear relationship between mach and altitude, velocity and altitude
- Possible exponential relationship between heat rate and Reynolds number.

Next, correlation matrixes were developed which specified the Pearson correlation and corresponding p-values. Given the inherent relationships between the independent or predictor variables, a principal components analysis was performed to help define a set of orthogonal variables so that the first principal component accounts for the largest possible amount of the total dispersion in the data, the second principal component accounts for the second largest possible amount of the total dispersion in the data, etc. This would be beneficial in helping to identify a subset list of candidate predictor variables for the analysis

Another method that was used to identify a subset list of candidate predictor variables is best subset selection. Best subset selection identified altitude, velocity, mach, dynamic pressure and Reynolds as the top five prediction variables. These are included in the regression model that is in the Appendix.

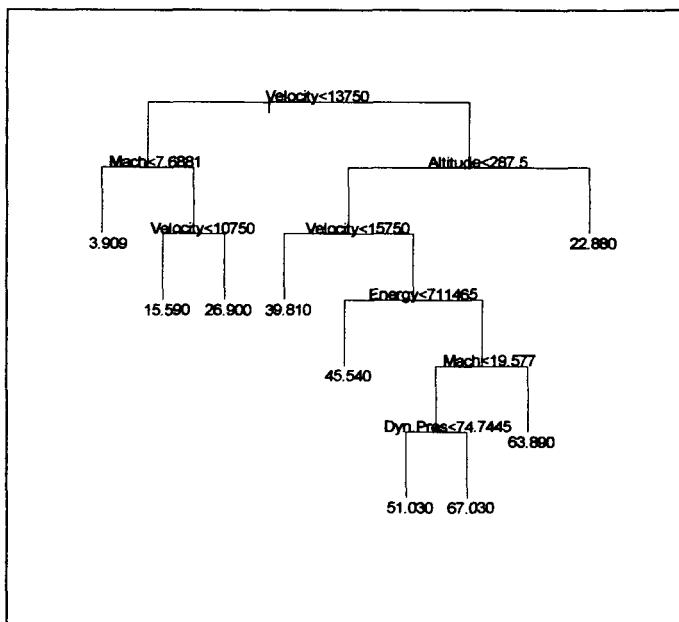
Classification and Regression Tree (CART) based models are exploratory techniques for uncovering structure in data that are used:

- To develop prediction rules that can be rapidly evaluated
- To screen variables
- To assess the adequacy of linear models
- To summarize large data sets for both classification and regression problems.

Figure 1 displays the resulting CART tree. CART selected velocity, mach, altitude, energy and dynamic pressure as the primary prediction variables. The tree indicates that for those data cases with velocity measurements less than 13750, the predicted values for

heat rate are generally below thirty. Furthermore, if values of mach are below 7.7, then the predicted heat rate is approximately 3.909.

Figure 1. Classification and Regression Tree for Corridor Data



The classical regression methods are often used to obtain models for prediction. The challenge is the development of the best mathematical expression to describe in some sense the behavior of a random variable of interest as a function of one or more independent or predictor variables. The classical regression techniques however make several strong assumptions about the underlying data, and the data can fail to satisfy these assumptions in several different ways as indicated in the Analysis Methods paragraph.

In the case where there are one or more outliers in the data or the data may not be fitted well by a linear model, robust regression methods come into play. This method minimizes the effect of the outliers and can be useful in helping to identify the outliers in the data.

Scatterplot smoothers are useful tools for fitting arbitrary smooth functions to a scatter plot of data points. The smoother summarizes the trend of the response as function of the predictor variables. All of the above analysis methods are used to explore the given data sets.

Results

Several approaches were used in the exploration and identification of statistical and mathematical models for the given data sets including the classical multiple regression, classification and regression trees (CART), and several graphical methods. One of the interesting results concerns a comparison of some initial multiple regression model types using only the independent predictor variables for both full and corridor data sets. These results are summarized below in Table A that includes Data, Coefficient of Determination (R^2), Adjusted R^2 , fit standard error S, F-statistics and the model type.

Table A: Comparison of Model Types for Full and Corridor Data using Three (3) Independent Predictor Variables

Data	R ²	Adj R ²	Std Error	F-statistic	Model
Full	48.3%	48.2%	196.5	394.15	Linear
Corridor	85.2%	84.9%	8.7	257.21	Linear
Full	84.4%	84.4%	108.0	1140.45	Quadratic
Corridor	97.6%	97.5	3.54	895.68	Quadratic
Full	85.6%	85.5	103.9	937.21	Cubic,Inter
Corridor	99.7%	99.6%	1.34	4751.89	Cubic,Inter

In reviewing Table A, a likely conclusion is that the regression models appear to be more appropriate for the corridor data than the full trajectory data sets for all model types.

A more in-depth analysis was conducted on the corridor data set as it simulates possible entry trajectory and heating rates of an experimental space vehicle. The structured approach that was used for model identification consists of the following: (1) analyze the summary statistics results for errors and consistency, (2) conduct analysis using only the independent predictor variables, (3) use graphical methods to identify underlying relationships, (4) employ methods (Best Subset Selection, Principal Components, etc..) which aid in identifying most likely additional predictor variables and (5) specify a model using classical regression, classification and regression trees (CART) and other statistical methods. The results are summarized in Table B below that includes rank, R^2 , adjusted R^2 , fit standard error (S), F-statistics and the model type. For illustrative purposes, Tables 1 and 2 and Figures 2 and 3 in the Appendix provide some of the graphical and regression modeling methods that were considered for model selection.

Table B: Identification of Model Types for the Corridor Data Set

Rank	R ²	Adj R ²	Std Error	F-statistic	Model
1	99.8	99.7	1.130	4140.87	Quad&Inter (5V)
2	99.7	99.6	1.348	4196.66	Cubic&Inter (3V)
3	99.4	99.4	1.724	3843.80	Linear (6V)
4	99.4	99.3	1.851	1665.11	Cubic WO Ind(7V)
5	99.1	99.0	2.209	2798.68	Linear 1 (5V)
6	97.6	97.5	3.54	895.68	Quad& Inter (3V)
7	96.77	—	4.1533	483.15	CART
8	85.2	84.9	8.72	257.21	Linear (3V)

Conclusions

A number of methods were considered in this analysis including classical multiple regression, polynomial regression, classification regression trees (CART), principal components, correlation matrix and residual analysis. Several graphical methods were used in model development and assessing model adequacy. In addition, several techniques were used to screen/identify underlying relationships. For example the matrix plots suggested the inclusion of quadratic and interaction terms in our models. On the other hand, principal components and best subset selection methods were used to screen and identify the main predictor variables. All of these methods were useful in guiding us in the selection of the predictor variables in our models. Using all of the above methods, several promising candidate models have been identified that may be used to predict the response variable, heat rate for the entry corridor data set. In the next phase of our work, validation of the adequacy of our models and other advanced methods will be explored.

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APPENDIX

Table 1. Regression Model Corridor Data (5V)

The regression equation is					
Heat Rate, BTU/ft ² /s = 66.3 - 0.871 Altitude, kft					
+ 0.0246 Velocity, ft/sec - 14.4 Mach - 0.162 Dyn. Pres. lb/ft ²					
+ 0.000054 Reynolds per ft					
Predictor	Coef	SE Coef	T	P	
Constant	66.274	5.196	12.76	0.000	
Altitude	-0.87060	0.03237	-26.89	0.000	
Velocity	0.0246292	0.0005425	45.40	0.000	
Mach	-14.4126	0.5654	-25.49	0.000	
Dyn. Pre	-0.16206	0.01120	-14.47	0.000	
Reynolds	0.00005438	0.00000767	7.09	0.000	
S = 2.209 R-Sq = 99.1% R-Sq(adj) = 99.0%					

Table 2. Analysis of Variance (5V)

Source	DF	SS	MS	F	P
Regression	5	68258	13652	2798.68	0.000
Residual Error	132	644	5		
Total	137	68902			

Figure 3. Normal Probability Plot (5V)

Normal Probability Plot of the Residuals
(response is Heat Rate)

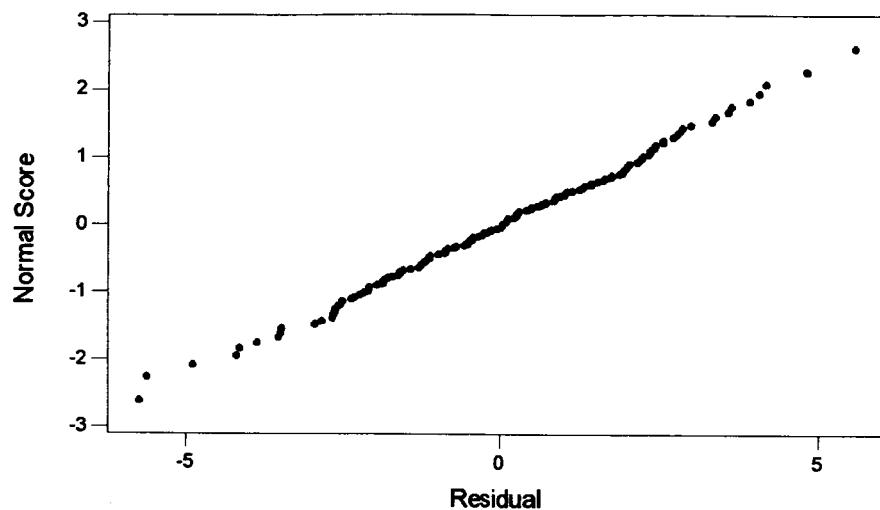


Figure 4. Residual Plot (5V)

Residuals Versus the Fitted Values
(response is Heat Rate)

